Electronic Supplementary Material for CrystEngComm

Supporting Information for

Silver isonicotinamide Frameworks Extended by arenedisulfonate via Coordination Bonds, Hydrogen bonds and Ag-Ag Interactions

Zhao-Xun Lian[1], **Jiwen Cai**[1, 2*], **Cai-Hong Chen**[1, 3]

1. *School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China*
2. *School of Pharmaceutical Sciences, Sun Yat-Sen University, Guangzhou 510080, People's Republic of China. puscjw@mail.sysu.edu.cn*
3. *School of Chemical Science, South China University of Technology, Guangzhou 510641, People's Republic of China*

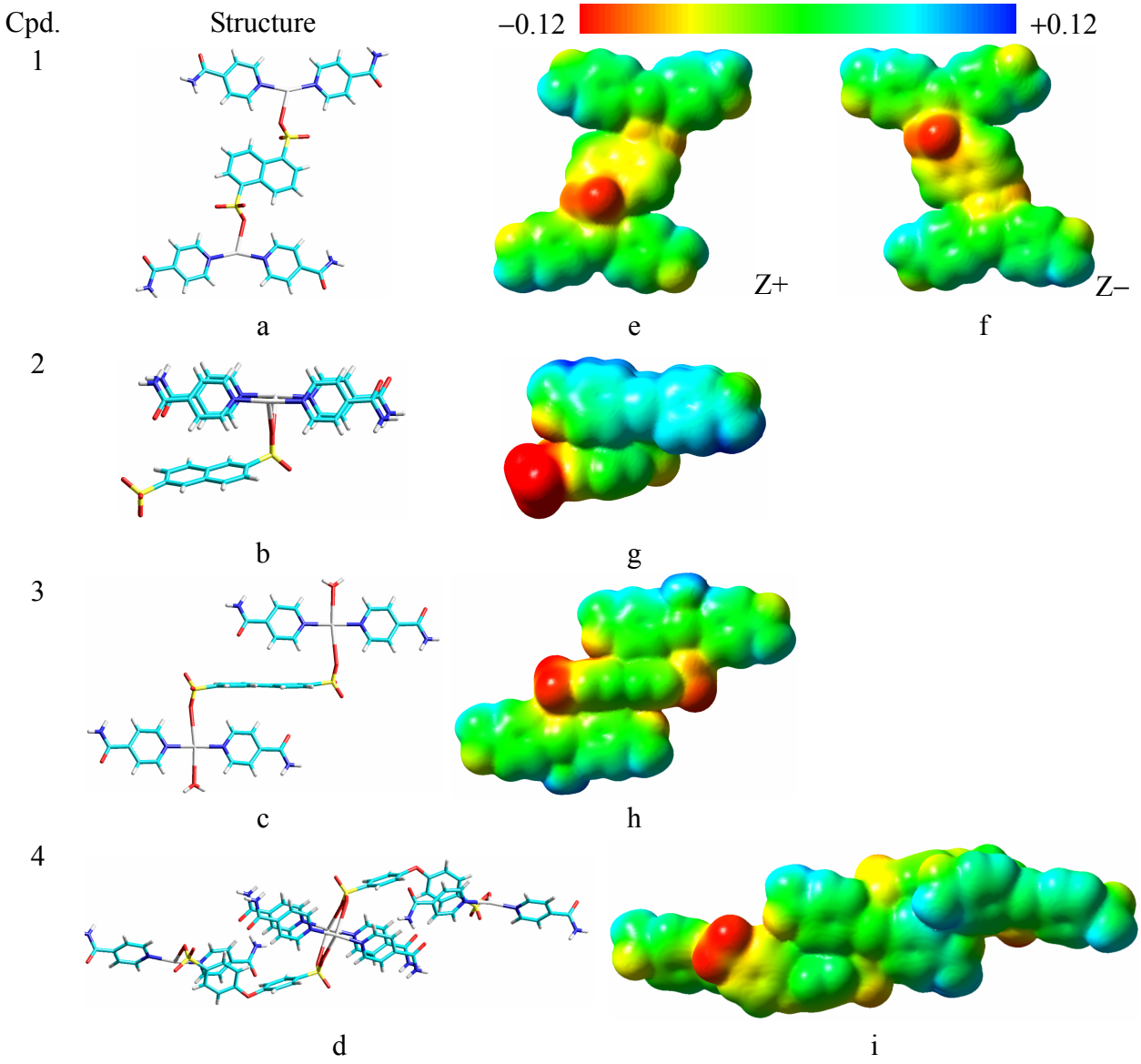

Figure S1. Calculated electrostatic potential (ESP) surfaces of the minimal units (single layer) for compounds **1-4** based on the crystal structures. The color.coded ESP is expressed as the potential energy felt by a probe of positive unit charge at a particular point in space. The ESP in the present work was calculated at the density functional theory (DFT)[1] B3LYP/3-21G level with ECP for the Ag atom from LANL2DZ using Gaussian 03[2] and being mapped on an isosurface of the total SCF electronic density at a value of 0.0004 au. The color bars range from red (electronegative) through green to blue (electropositive) with the mapped ESP values from –0.12 to +0.12 hartrees linearly. In (e) and (f), the ESP surfaces for compound **1** were displayed separately along the two Cartesian directions (Z+ and Z–).

References

1. D. Becke. *J. Chem. Phys*. 1993, **98**, 5648.

2. M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, Jr.T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian 03 (C.02), Gaussian, Inc. Wallingford CT, 2004.